

Nitrogen-containing species in the structure of the synthesized nano-hydroxyapatite

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Abstract

Synthesized by the wet chemical precipitation technique, hydroxyapatite (HAp) powders with the sizes of the crystallites of 20-50 nm and 1 μm were analyzed by different analytical methods. By means of electron paramagnetic resonance (EPR) it is shown that during the synthesis process nitrate anions from the reagents (byproducts) could incorporate into the HAp structure. The relaxation times and EPR parameters of the stable axially symmetric NO₃²⁻ paramagnetic centers detected after X-ray irradiation are measured with high accuracy. Analyses of high-frequency (95 GHz) electron-nuclear double resonance spectra from ¹H and ³¹P nuclei and ab initio density functional theory calculations allow suggesting that the paramagnetic centers and nitrate anions as the precursors of NO₃²⁻ radicals preferably occupy PO₄³⁻ site in the HAp structure. © 2014 Pleiades Publishing, Inc.

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